Varieties of Signature Tensors
Lecture #1

Carlos Enrique Améndola Cerón
(TU Munich)

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Setup: Signatures

- Let $X : [0,1] \to \mathbb{R}^d$ be a piecewise differentiable path.
- Coordinate functions: $X_1, X_2, \ldots, X_d : \mathbb{R} \to \mathbb{R}$
- Their differentials $\mathrm{d}X_i(t) = X_i'(t)\mathrm{d}t$ are the coordinates of the vector

$$\mathrm{d}X = (\mathrm{d}X_1, \mathrm{d}X_2, \ldots, \mathrm{d}X_d)$$

- The kth signature of X is a **tensor** $\sigma^{(k)}(X)$ of order k and format $d \times d \times \cdots \times d$. It is the multivariate integral:

$$\sigma^{(k)}(X) \;=\; \int_\Delta \mathrm{d}X(t_1) \otimes \mathrm{d}X(t_2) \otimes \cdots \otimes \mathrm{d}X(t_k),$$

where $\Delta = \left\{(t_1, t_2, \ldots, t_k) \in \mathbb{R}^k : 0 \leq t_1 \leq t_2 \leq \cdots \leq t_k \leq 1\right\}$.

- Its d^k entries $\sigma_{i_1 i_2 \ldots i_k}$ are the *iterated integrals*

$$\sigma_{i_1 i_2 \cdots i_k} = \int_0^1 \int_0^{t_k} \cdots \int_0^{t_3} \int_0^{t_2} \mathrm{d}X_{i_1}(t_1)\, \mathrm{d}X_{i_2}(t_2) \cdots \mathrm{d}X_{i_k}(t_k).$$

Signatures

- $\sigma^{(k)}(X)$ has entries

$$\sigma_{i_1 i_2 \cdots i_k} = \int_0^1 \int_0^{t_k} \cdots \int_0^{t_3} \int_0^{t_2} \mathrm{d}X_{i_1}(t_1)\, \mathrm{d}X_{i_2}(t_2) \cdots \mathrm{d}X_{i_k}(t_k).$$

- Let's start with $k = 1$:
- Fundamental Theorem of Calculus:

$$\int_0^1 \mathrm{d}X_i(t) = X_i(1) - X_i(0)$$

- The first signature of the path X is

$$\sigma^{(1)}(X) = \int_0^1 \mathrm{d}X(t) = X(1) - X(0) \in \mathbb{R}^d$$

Signature Matrices

- Now let's consider $k = 2$. Then the second signature $S = \sigma^{(2)}(X)$ is the $d \times d$ matrix with entries

$$\sigma_{ij} = \int_0^1 \int_0^t \mathrm{d}X_i(s)\mathrm{d}X_j(t)$$

- Set $X(0) = 0$. Applying Fundamental Theorem of Calculus again:

$$\sigma_{ij} = \int_0^1 X_i(t)X_j'(t)\mathrm{d}t$$

- We obtain

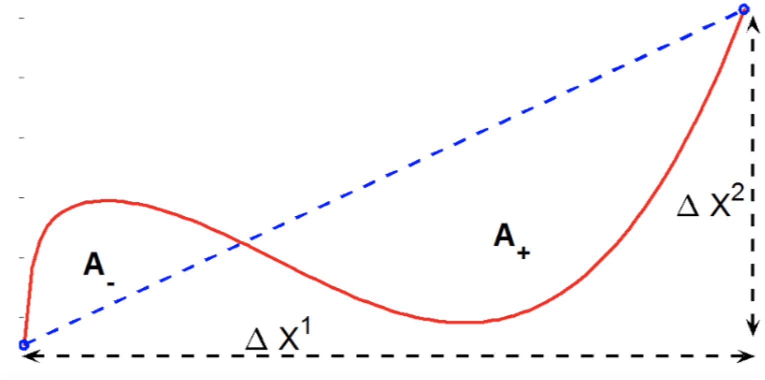
$$\sigma_{ij} + \sigma_{ji} = X_i(1) \cdot X_j(1)$$

- In matrix notation, $S + S^T = X(1) \cdot X(1)^T$
- In particular, the symmetric matrix $S + S^T$ has rank one!
- The skew-symmetric matrix $S - S^T$ measures *deviation from linearity*:

$$\sigma_{ij} - \sigma_{ji} = \int_0^1 (X_i(t)X_j'(t) - X_j(t)X_i'(t))\mathrm{d}t$$

Lévy Area

The entry $\sigma_{ij} - \sigma_{ji}$ of the skew-symmetric matrix $S - S^T$ is the area below the line minus the area above the line, known as a Lévy area:



Some History

- Introduced by Kuo Tsai Chen in the 1950s:
  K.-T. Chen: *Integration of paths, geometric invariants and a generalized Baker-Hausdorff formula*, Annals of Mathematics **65** (1957)
  K.-T. Chen: *Integration of paths a faithful representation of paths by noncommutative formal power series*, Transactions AMS **89** (1958)
- The *signature* of a path X is the sequence of tensors

$$\sigma(X) = \big(1, \sigma^{(1)}(X), \sigma^{(2)}(X), \sigma^{(3)}(X), \ldots, \sigma^{(n)}(X), \ldots\big)$$

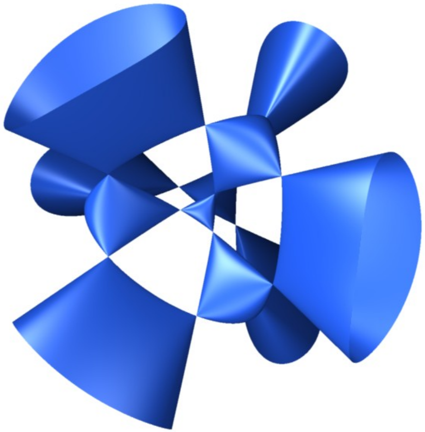
- *Essential question*: how much information does the signature reveal about the path X?
- Signature determines paths! (modulo starting point, parametrization and tree-like excursion)
  B. Hambly and T. Lyons: *Uniqueness for the signature of a path of bounded variation and the reduced path group*, Annals of Mathematics **171** (2010)

History

- Signatures are central to the theory of rough paths, a revolutionary view on *Stochastic Analysis*.
- P. Friz and N. Victoir: *Multidimensional Stochastic Processes as Rough Paths*. Theory and Applications, Cambridge University Press, 2010.
  P. Friz and M. Hairer: *A Course on Rough Paths. With an introduction to regularity structures*, Universitext, Springer, Cham, 2014.
- They can be used to encode and model data!
  T. Lyons: *Rough paths, signatures and the modelling of functions on streams*, Proc. International Congress of Mathematicians 2014, Seoul
  I. Chevyrev and A. Kormilitzin: *A primer on the signature method in machine learning*, arXiv:1603.03788.

Present...and Future

- What happens when signatures meet Algebraic Statistics?
- C. Améndola, P. Friz and B. Sturmfels: *Varieties of Signature Tensors*, arXiv:1804.08325.
- M. Pfeffer, A. Seigal and B. Sturmfels: *Learning Paths from Signature Tensors*, arXiv:1809.01588.
- F. Galuppi: *The Rough Veronese Variety*, arXiv:1809.02522.
- L. Colmenajero and M. Michalek: *Signature Varieties of Axis Paths*, in preparation.
- *YOUR papers on signatures!*
- We are interested in projective varieties in tensor space $\mathbb{P}^{d^k-1}$ that arise when X ranges over some nice families of paths.



$$x^4 + y^4 + z^4 - x^2 - y^2 - z^2 - x^2y^2 - x^2z^2 - y^2z^2 + 1 = 0$$

Algebraic Varieties

- Solution set of a polynomial system of equations.
- $\mathcal{V} \subseteq K^d$ (affine) algebraic variety $\Rightarrow$ we can find a set of polynomials $F \subseteq \mathbb{K}[s_1, \ldots, s_d]$ such that

$$\mathcal{V} = \{a \in \mathbb{K}^d | f(a) = 0 \text{ for all } f \in \mathcal{F}\}$$

- If polynomials are homogeneous $\Rightarrow$ work in projective space $\mathbb{P}^{d-1}$.
- The ideal V associated to a variety $\mathcal{V}$: set of all polynomials that vanish on $\mathcal{V}$.
- Key Fact: a polynomial map $\sigma : \mathbb{K}^m \to \mathbb{K}^d$ induces naturally an algebraic variety that contains the image of σ.

Example of a Signature Variety

- Let $d = 2$ and consider quadratic paths in the plane $\mathbb{R}^2$:

$$X(t) = \left(x_{11}t + x_{12}t^2,\ x_{21}t + x_{22}t^2\right)^T = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \cdot \begin{pmatrix} t \\ t^2 \end{pmatrix}$$

- Their kth signature tensors depend *polynomially* of degree k on x_{ij}.
- $\sigma^{(1)}(X) = (\sigma_1, \sigma_2) = \left(x_{11} + x_{12}, x_{21} + x_{22}\right)$.
-

$$\begin{aligned} \sigma_{ij} &= \int_0^1 \int_0^t (x_{i1} + 2x_{i2}s)\mathrm{d}s\,(x_{j1} + 2x_{j2}t)\mathrm{d}t \\ &= \int_0^1 \left(x_{i1}t + x_{i2}t^2\right)\left(x_{j1} + 2x_{j2}t\right)\mathrm{d}t \\ &= \int_0^1 [x_{i1}x_{j1}t + (2x_{i1}x_{j2} + x_{i2}x_{j1})t^2 + 2x_{i2}x_{j2}t^3]\,\mathrm{d}t \\ &= \tfrac{1}{2}x_{i1}x_{j1} + \tfrac{2}{3}x_{i1}x_{j2} + \tfrac{1}{3}x_{i2}x_{j1} + \tfrac{1}{2}x_{i2}x_{j2}. \end{aligned}$$

- We can write $\sigma^{(2)}(X)$ as

$$\frac{1}{2}\begin{pmatrix} x_{11}+x_{12} \\ x_{21}+x_{22} \end{pmatrix}\left(x_{11}+x_{12},\ x_{21}+x_{22}\right) + \frac{1}{6}(x_{11}x_{22} - x_{12}x_{21})\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Example of a Signature Variety

- The variety of all such signature matrices is the solution set of the quadratic equation

$$(\sigma_{12} + \sigma_{21})^2 - 4\sigma_{11}\sigma_{22} \ = \ 0.$$

- This means that the image variety associated to signature matrices of polynomial paths of degree two in the plane is a hypersurface in $\mathbb{P}^3$.
- We will denote this surface by $\mathcal{P}_{2,2,2}$. Its prime ideal generated by the quadric above is $P_{2,2,2}$.
- We want to study and *understand* these varieties!
- Question: What is the resulting variety if we restrict to linear paths?
- *Answer*: The *Veronese* variety!

- The third signature $\sigma^{(3)}(X)$ is a $2 \times 2 \times 2$-tensor ($d = 2, k = 3$).

$$
\begin{array}{rcccc}
\sigma_{111} & = & \frac{1}{6}(x_{11} + x_{12})^3 & & \\
\sigma_{112} & = & \frac{1}{6}(x_{11}+x_{12})^2(x_{21}+x_{22}) & + & \frac{1}{60}(5x_{11} + 4x_{12})(x_{11}x_{22} - x_{12}x_{21}) \\
\sigma_{121} & = & \frac{1}{6}(x_{11}+x_{12})^2(x_{21}+x_{22}) & + & \frac{1}{60}(2x_{12})(x_{11}x_{22} - x_{12}x_{21}) \\
\sigma_{211} & = & \frac{1}{6}(x_{11}+x_{12})^2(x_{21}+x_{22}) & - & \frac{1}{60}(5x_{11} + 6x_{12})(x_{11}x_{22} - x_{12}x_{21}) \\
\sigma_{122} & = & \frac{1}{6}(x_{11}+x_{12})(x_{21}+x_{22})^2 & + & \frac{1}{60}(5x_{21} + 6x_{22})(x_{11}x_{22} - x_{12}x_{21}) \\
\sigma_{212} & = & \frac{1}{6}(x_{11}+x_{12})(x_{21}+x_{22})^2 & - & \frac{1}{60}(2x_{22})(x_{11}x_{22} - x_{12}x_{21}) \\
\sigma_{221} & = & \frac{1}{6}(x_{11}+x_{12})(x_{21}+x_{22})^2 & - & \frac{1}{60}(5x_{21} + 4x_{22})(x_{11}x_{22} - x_{12}x_{21}) \\
\sigma_{222} & = & \frac{1}{6}(x_{21} + x_{22})^3 & &
\end{array}
$$

- Goal: find the polynomial relations among the eight entries of $\sigma^{(3)}(X)$
- Image signature variety is $\mathcal{P}_{2,3,2}$ and its prime ideal is $P_{2,3,2}$.
- An instance of the general $P_{d,k,m}$ of polynomial paths of degree m.

Some Favorite Tensors

- The *canonical axis path* C_{axis} in $\mathbb{R}^d$ goes from $(0,0,\ldots,0)$ to $(1,1,\ldots,1)$ in d linear steps in unit directions $e_1, e_2, \ldots, e_d$.
  `Exercise`: What is $\sigma^{(k)}(C_{\mathrm{axis}})$?
  Hint: The entry $\sigma_{i_1 i_2 \ldots i_k}$ is always zero unless $i_1 \leq i_2 \leq \cdots \leq i_k$.
- The *canonical monomial path* C_{mono} in $\mathbb{R}^d$ given by $t \to (t, t^2, t^3, \ldots, t^d)$ goes from $(0,0,\ldots,0)$ to $(1,1,\ldots,1)$ along the rational normal curve.
  `Exercise`: What is $\sigma^{(k)}(C_{\mathrm{mono}})$?
- *Key observation*: We can compute the kth signature tensors of piecewise linear paths or polynomial paths just by knowing $\sigma^{(k)}(C_{axis})$ or $\sigma^{(k)}(C_{\mathrm{mono}})$, respectively.
- *How?* Encode any such path as a matrix $\mathbf{X}$. The map $X \to \sigma^{(k)}(X)$ is then given by the congruence action $\mathbf{X} \to \mathbf{X} \cdot [\![C; \mathbf{X}, \mathbf{X}, \ldots, \mathbf{X}]\!]$.

The Congruence Action: Example

Example ($\mathcal{P}_{2,2,2}$ revisited)

Consider again quadratic paths in $\mathbb{R}^2$ that were given by

$$X(t) = \left(x_{11}t + x_{12}t^2,\ x_{21}t + x_{22}t^2\right)^T = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \cdot \begin{pmatrix} t \\ t^2 \end{pmatrix} = \mathbf{X} \cdot \begin{pmatrix} t \\ t^2 \end{pmatrix}$$

The core tensor is the signature matrix $\sigma^{(2)}(C_{mono}) = \begin{pmatrix} \frac{1}{2} & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{2} \end{pmatrix}$.

Then $\sigma^{(2)}(X)$ is given by $[\![C; \mathbf{X}, \mathbf{X}]\!] = \mathbf{X} \cdot \sigma^{(2)}(C_{mono}) \cdot \mathbf{X}^{\mathbf{T}}$
Indeed, we had computed that

$$\sigma_{ij}(X) = \frac{1}{2}x_{i1}x_{j1} + \frac{2}{3}x_{i1}x_{j2} + \frac{1}{3}x_{i2}x_{j1} + \frac{1}{2}x_{i2}x_{j2}.$$

The Skyline Path

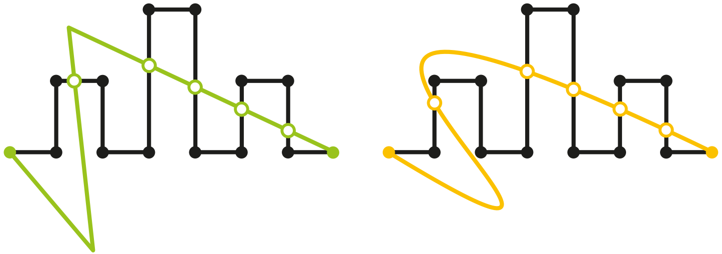
is an axis path with 13 steps in $\mathbb{R}^2$, given by the columns of:

$$\mathbf{X} = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 & 0 & 2 & 0 & -2 & 0 & 1 & 0 & -1 & 0 \end{bmatrix}.$$

Its $2 \times 2 \times 2$ signature tensor can be obtained by multiplying the core tensor C_{axis} of format $13 \times 13 \times 13$ with the 2×13 matrix $\mathbf{X}$ on all three sides:

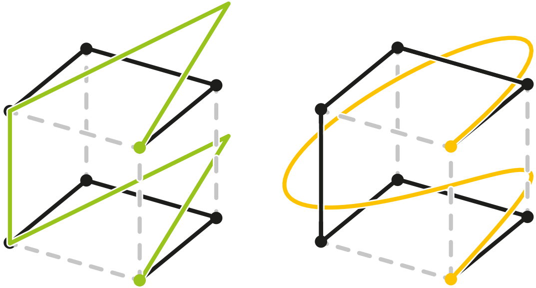
$$S_{\text{skyline}} = [\![C_{\text{axis}}; \mathbf{X}, \mathbf{X}, \mathbf{X}]\!] = \frac{1}{6} \left[\begin{array}{cc|cc} 343 & 0 & -84 & 18 \\ 84 & 18 & -36 & 0 \end{array} \right].$$

Three-step path and cubic path with the same signature tensor:



Klee-Minty Path

$$\mathbf{X} = \begin{bmatrix} 1 & 0 & -1 & 0 & 1 & 0 & -1 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}.$$



$$\sigma^{(3)}(X) = [\![C_{\mathrm{axis}}; \mathbf{X}, \mathbf{X}, \mathbf{X}]\!] = \frac{1}{6} \left[\begin{array}{ccc|ccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & -6 & -6 & 3 & 3 \\ 0 & 6 & 0 & -6 & 3 & -3 & 0 & 0 & 1 \end{array} \right]$$